

Ridge Regression

Nipun Batra

July 26, 2025

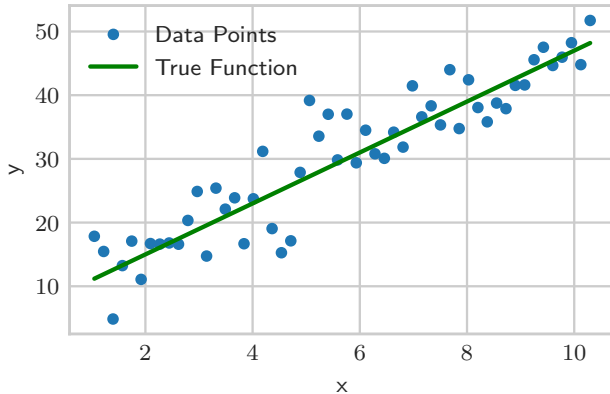
IIT Gandhinagar

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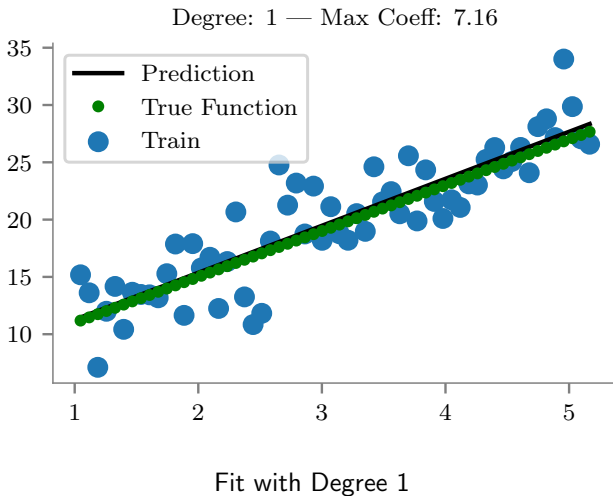
In $f(x) = c_0 + c_1x + c_2x^2 + \dots$ it is $\max |c_i|$

Introduction

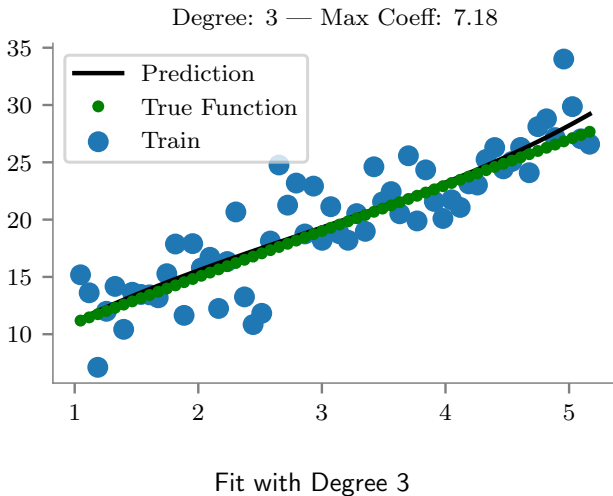


Base Data Set

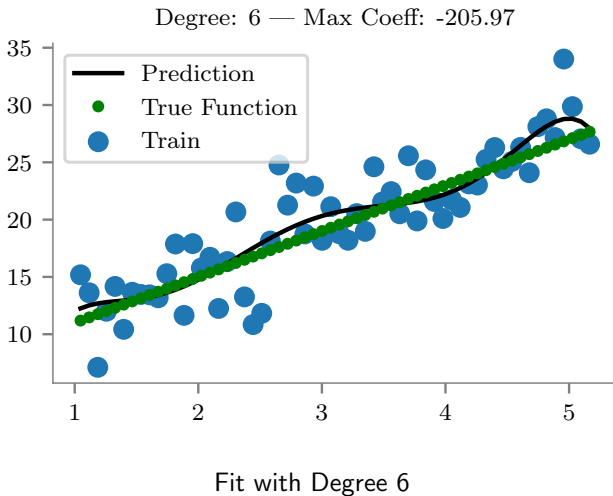
Introduction



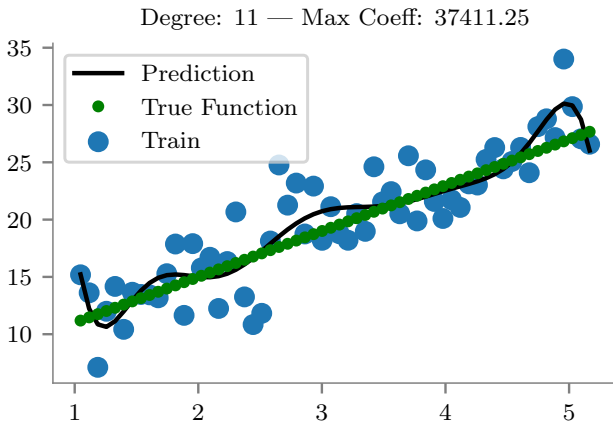
Introduction



Introduction



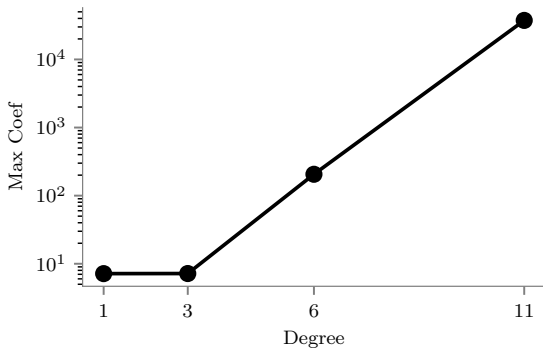
Introduction



Fit with Degree 11

Introduction

In the examples we notice that as the degree increases (as the prediction starts to overfit the base data), the maximum coefficient also increases.



Trend of the coefficients

To prevent overfitting we place penalties on large θ_i

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Objective:

$$\begin{aligned} &\text{Minimise } (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) \\ &\text{s.t. } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq S \end{aligned}$$

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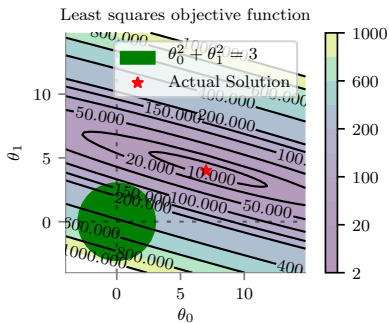
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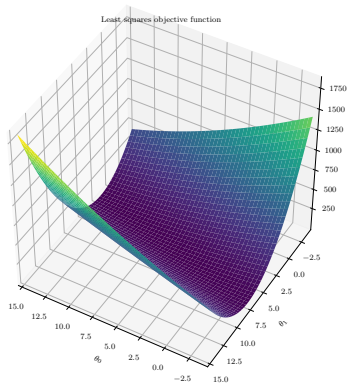
This is equivalent to

$$\text{Minimise } (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \delta^2 \boldsymbol{\theta}^T \boldsymbol{\theta}$$

Introduction



(a) Contour Plot



(b) Surface Plot

Visualization of the Example

To implement this we use KKT Conditions

KKT Conditions

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$$\text{Minimise } (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})$$

$$\text{s.t. } \boldsymbol{\theta}^T \boldsymbol{\theta} \leq S$$

$$L(\boldsymbol{\theta}, \mu) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^T (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \mu (\boldsymbol{\theta}^T \boldsymbol{\theta} - S)$$

where, $\mu \geq 0$ (and $\mu = \delta^2$)

KKT Conditions

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If $\mu = 0$

There is no regularization

No effect on constraint

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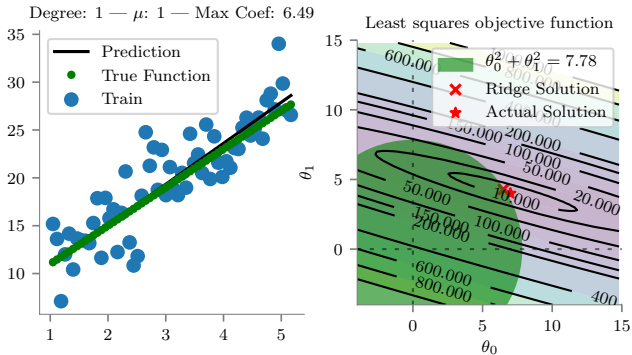
There is no regularization

No effect on constraint

If $\mu \neq 0$

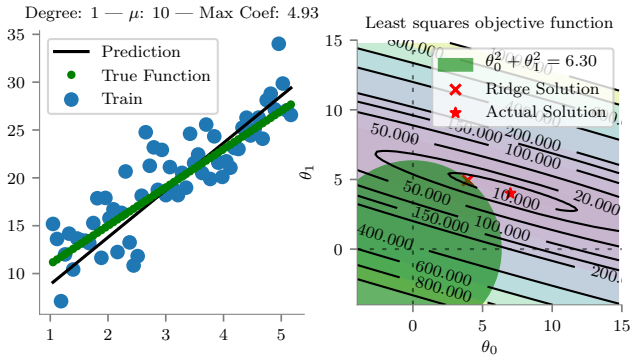
$$\implies \boldsymbol{\theta}^T \boldsymbol{\theta} - S = 0$$

Effect of μ



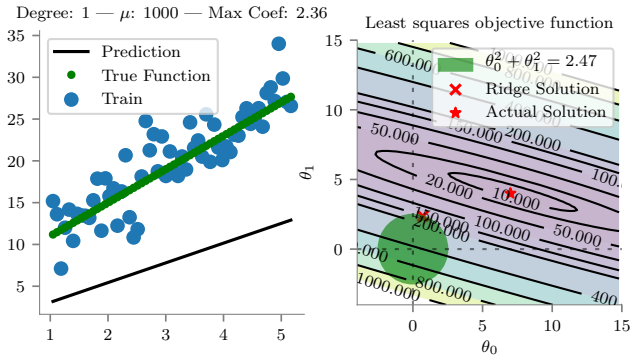
$$\mu = 1$$

Effect of μ



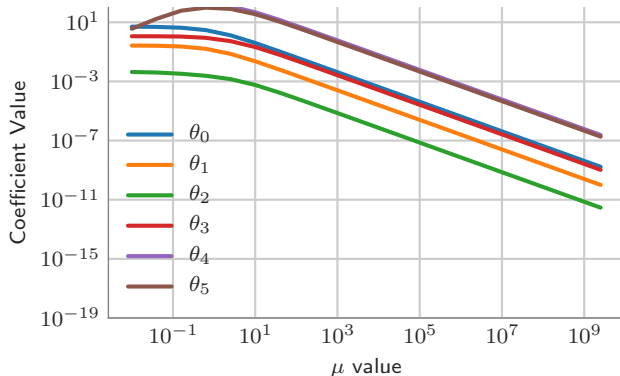
$$\mu = 10$$

Effect of μ



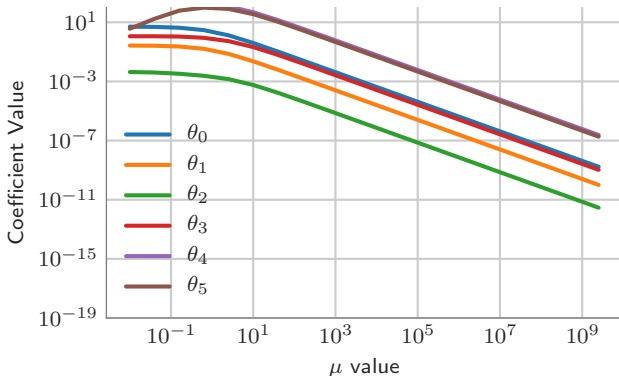
$$\mu = 1000$$

Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ
(on the *Real Estate Data Set*)

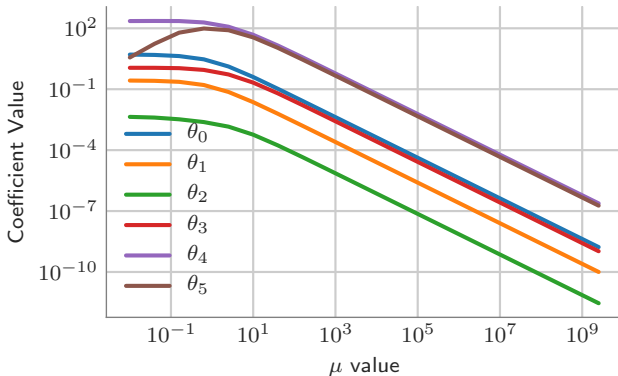
Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ
(on the *Real Estate Data Set*)

Are θ_i all zero for high μ ?

Effect of μ - Regularization of Parameters



Comparing the magnitudes of the coefficients with varying μ
(on the *Real Estate Data Set*)

Ridge Objective:

$$\min_{\theta} (\mathbf{y} - \mathbf{X}\theta)^T (\mathbf{y} - \mathbf{X}\theta) + \mu \theta^T \theta$$

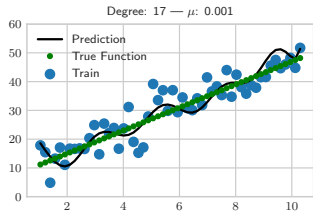
$$\frac{\partial L(\theta, \mu)}{\partial \theta} = 0$$

$$\frac{\partial}{\partial \theta} \left\{ \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{X}\theta + \theta^T \mathbf{X}^T \mathbf{X}\theta \right\} + \frac{\partial}{\partial \theta} \mu \theta^T \theta = 0$$

$$\implies -\mathbf{X}^T \mathbf{y} + (\mathbf{X}^T \mathbf{X} + \mu \mathbf{I}) \theta = 0$$

$$\implies \theta^* = (\mathbf{X}^T \mathbf{X} + \mu \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y}$$

Bias/Variance

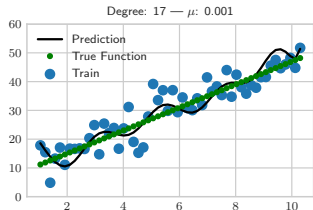


Fit High Order Polynomial

\implies high variance

$\implies \mu \rightarrow 0$

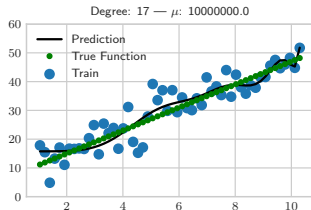
Bias/Variance



Fit High Order Polynomial

\Rightarrow high variance

$\Rightarrow \mu \rightarrow 0$



Fit High Order Polynomial

\Rightarrow low variance

$\Rightarrow \mu \rightarrow \infty$

Example

Q.) Solve Regularized ($\mu = 2$) and Unregularized.

Example: Unregularised

$$\theta = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{y})$$

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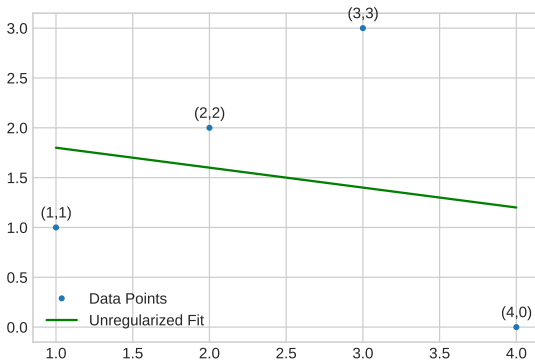
$$\mathbf{X}^T \mathbf{X} = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix}$$

$$(\mathbf{X}^T \mathbf{X})^{-1} = \frac{1}{20} \begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}$$

$$\mathbf{X}^T \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Example: Unregularised

$$\theta = (\mathbf{X}^T \mathbf{X})^{-1} (\mathbf{X}^T \mathbf{y})$$
$$\begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} 2 \\ -1/5 \end{bmatrix}$$



Example: Regularised

$$\theta = (\mathbf{X}^T \mathbf{X} + \mu \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y})$$

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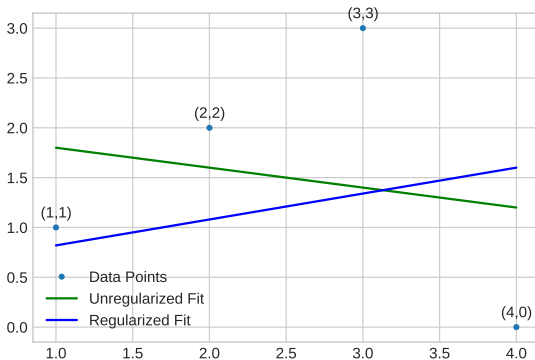
$$\mathbf{X}^T \mathbf{X} + \mu \mathbf{I} = \begin{bmatrix} 6 & 10 \\ 10 & 32 \end{bmatrix}$$

$$(\mathbf{X}^T \mathbf{X} + \mu \mathbf{I})^{-1} = \frac{1}{92} \begin{bmatrix} 32 & -10 \\ -10 & 6 \end{bmatrix}$$

$$\mathbf{X}^T \mathbf{y} = \begin{bmatrix} 6 \\ 14 \end{bmatrix}$$

Example: Regularised

$$\theta = (\mathbf{X}^T \mathbf{X} + \mu \mathbf{I})^{-1} (\mathbf{X}^T \mathbf{y})$$
$$\begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix} = \begin{bmatrix} 0.56 \\ 0.26 \end{bmatrix}$$



Multi-collinearity

$(\mathbf{X}^T \mathbf{X})^{-1}$ is not computable when $|\mathbf{X}^T \mathbf{X}| = 0$.

This was a drawback of using linear regression

$$\mathbf{X} = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 2 & 4 \\ 1 & 3 & 6 \end{bmatrix}$$

The matrix \mathbf{X} is not full rank.

Multi-collinearity

But with ridge regression, the matrix to be inverted is $\mathbf{X}^T\mathbf{X} + \mu\mathbf{I}$ and not $\mathbf{X}^T\mathbf{X}$.

$$\mathbf{X}^T\mathbf{X} + \mu\mathbf{I} = \begin{bmatrix} 3 + \mu & 6 & 12 \\ 6 & 14 + \mu & 28 \\ 12 & 28 & 56 + \mu \end{bmatrix}$$

The matrix $\mathbf{X}^T\mathbf{X}$ would be full rank for $\mu > 0$.

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Another interpretation of “regularisation”

Extension of the analytical model

For ridge with no penalty on θ_0

$$\hat{\boldsymbol{\theta}} = \left(\mathbf{X}^T \mathbf{X} + \mu \mathbf{I}^* \right)^{-1} \mathbf{X}^T \mathbf{y}$$

where,

$$\mathbf{I}^* = \begin{bmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}$$

Ridge Solution using Gradient Descent

- $\theta = \theta - \alpha \frac{\partial}{\partial \theta} ((\mathbf{y} - \mathbf{X}\theta)^\top (\mathbf{y} - \mathbf{X}\theta) + \mu \theta^\top \theta)$

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- $\theta = \theta - \alpha (-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\theta + 2\mu \mathbf{I}\theta)$

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- $\theta = (1 - 2\alpha\mu \mathbf{I})\theta - \alpha (-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\theta)$

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- $\theta = \underbrace{(1 - 2\alpha\mu \mathbf{I})\theta}_{\text{Shrinking } \theta} - \alpha (-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\theta)$

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- Contrast with update equation for unregularised regression:

Ridge Solution using Gradient Descent

- $\theta = \theta - \alpha \frac{\partial}{\partial \theta} ((\mathbf{y} - \mathbf{X}\theta)^\top (\mathbf{y} - \mathbf{X}\theta) + \mu \theta^\top \theta)$
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- Contrast with update equation for unregularised regression:
- $\theta = \underbrace{\theta}_{\text{No Shrinking } \theta} - \alpha (-2\mathbf{X}^\top \mathbf{y} + 2\mathbf{X}^\top \mathbf{X}\theta)$